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COMPARISON OF THE ″TBD″ TOKEN MODEL TO AVAILABLE COMPETITORS

CFD code to model aerosol flows on a large scale. Whereas DNS is the proper way to calculate flows on the scale of turbulent eddies, computers are still a long way away from being powerful enough to calculate flows in practical industrial and environmental systems.

We have been developing a tool for the calculation of aerosol flows with the focus on the speed to reach the steady-state, efficiency and numerical accuracy.

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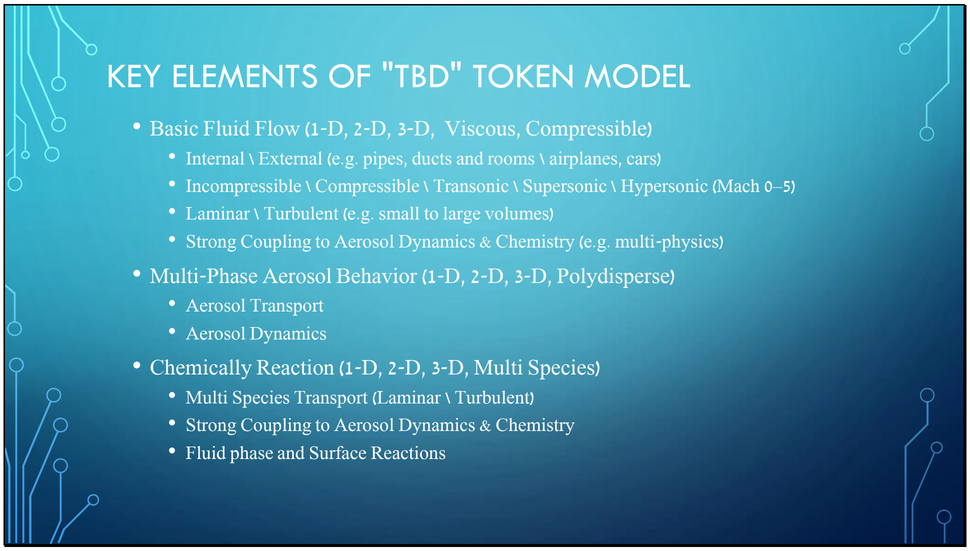

KEY ELEMENTS OF "TBD" TOKEN MODEL

- Basic Fluid Flow (1-D, 2-D, 3-D, Viscous, Compressible)
  - Internal \ External (e.g. pipes, ducts and rooms \ airplanes, cars)
  - Incompressible \ Compressible \ Transonic \ Supersonic \ Hypersonic (Mach 0–5)
  - Laminar \ Turbulent (e.g. small to large volumes)
  - Strong Coupling to Aerosol Dynamics & Chemistry (e.g. multi-physics)
- Multi-Phase Aerosol Behavior (1-D, 2-D, 3-D, Polydisperse)
  - Aerosol Transport
  - Aerosol Dynamics
- Chemically Reaction (1-D, 2-D, 3-D, Multi Species)
  - Multi Species Transport (Laminar \ Turbulent)
  - Strong Coupling to Aerosol Dynamics & Chemistry
  - Fluid phase and Surface Reactions

The basic elements of the model are shown here. In order to simulate these a wide variety of cases, the coupled model has been made as general as possible. The model consists three modules ...

PROVEN "TBD" TOKEN APPLICATIONS

- Prediction/Minimazation of Atmospheric Deposition
- Prediction/Minimazation of Heat Exchanger Fouling
- Aerosol Control in Nuclear Reactors
- Design of Particle Characterization Equipment
- Design of Dry Particle Inhalers
- Design of Nebulizer Pulmonary Drug Delivery Systems
- Design of Photocatalytic and Optical Particle Synthesis Processes
- Design of High Surface Area Metal Catalyst Particle Synthesis Processes Design of Nanostructured Doped Silica Particles for Fiber Optic Preform Manufacture.
- Design of Gas Phase Catalyst Synthesis Processes
- Design of Carbon Nanotubes and Nano Onions Synthesis Processes
- Design of Nanostructured Inhalable Drug and Drug Carrier Particle Synthesis Processes
- Design of Nano-drug Particle Synthesis Processes
- Design of Nano-particle Deposition Process
- Etc.

We have chosen to address two very different kinds of problems with this model to exemplify its generality. A brief background of these cases will be discussed... Aerosol Deposition in Combined Cycle Gas Turbines, and Aerosol formation and evolution in HSCT Nozzles and Plumes.

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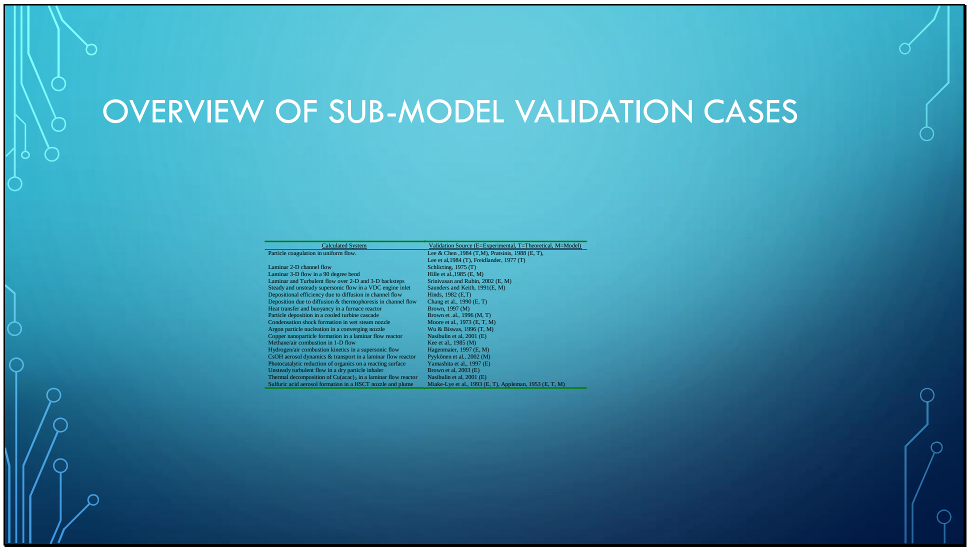

OVERVIEW OF SUB-MODEL VALIDATION CASES

Calculated System	Validation Source (E=Experimental, T=Theoretical, M=Model)
Particle coagulation in uniform flow.	Lee & Chen ,1984 (T,M), Pratsinis, 1988 (E, T), Lee et al,1984 (T), Freidlander, 1977 (T)
Laminar 2-D channel flow	Schlicting, 1975 (T)
Laminar 3-D flow in a 90 degree bend	Hille et al.,1985 (E, M)
Laminar and Turbulent flow over 2-D and 3-D backsteps	Srinivasan and Rubin, 2002 (E, M)
Steady and unsteady supersonic flow in a VDC engine inlet	Saunders and Keith, 1991(E, M)
Depositional efficiency due to diffusion in channel flow	Hinds, 1982 (E,T)
Deposition due to diffusion & thermophoresis in channel flow	Chang et al., 1990 (E, T)
Heat transfer and buoyancy in a furnace reactor	Brown, 1997 (M)
Particle deposition in a cooled turbine cascade	Brown et .al., 1996 (M, T)
Condensation shock formation in wet steam nozzle	Moore et al., 1973 (E, T, M)
Argon particle nucleation in a converging nozzle	Wu & Biswas, 1996 (T, M)
Copper nanoparticle formation in a laminar flow reactor	Nasibulin et al, 2001 (E)
Methane/air combustion in 1-D flow	Kee et al., 1985 (M)
Hydrogen/air combustion kinetics in a supersonic flow	Hagenmaier, 1997 (E, M)
CsOH aerosol dynamics & transport in a laminar flow reactor	Pyykönen et al., 2002 (M)
Photocatalytic reduction of organics on a reacting surface	Yamashita et al., 1997 (E)
Unsteady turbulent flow in a dry particle inhaler	Brown et al, 2003 (E)
Thermal decomposition of Cu(acac)$_2$ in a laminar flow reactor	Nasibulin et al, 2001 (E)
Sulfuric acid aerosol formation in a HSCT nozzle and plume	Miake-Lye et al., 1993 (E, T), Appleman, 1953 (E, T, M)

For example, the governing equations for a fluid flow can be written as a function of implicit primitive variables ρ, p, H and V as well as explicit variables μ, γ, k and MW. Chemical reactions and aerosol behavior can alter these quantities through various mechanisms.
With regard to gas phase, for instance, reactions can absorb or release thermal energy thus changing enthalpy and pressure or altered species concentrations can change the ρ , MW, and μ. A change in any such parameter can thus effect on the overall flow.
Additionally, the presence of aerosols in a flow can create strong coupling effects. The formation of aerosols through condensation and nucleation of species, for instance, can release thermal energy, effecting state variables, OR large number of volume concentrations of aerosols can effect the effective viscosity of the fluid.
Coupling in the reverse direction can also occur. Expansion of flow can alter saturation ratios leading to formation of aerosols, changing species concentrations and drive chemical reactions.
Obviously these coupling effects can become quite involved. In two and three dimensions, additional factors due to spatial variation of parameters complicate the process even further.
This presentation details and applies a method of modeling this intricate coupled behavior.
Solutions presented today will focus on the coupling of fluid and gas phase species concentrations on aerosol behavior where reverse coupling is weak. When complete, the model will be able to model coupling in detail.

Tow problems where this kind of coupling is important, namely:
Aerosol deposition in Gas Turbines, and Pollutant Formation in HSCT Nozzles and Plumes

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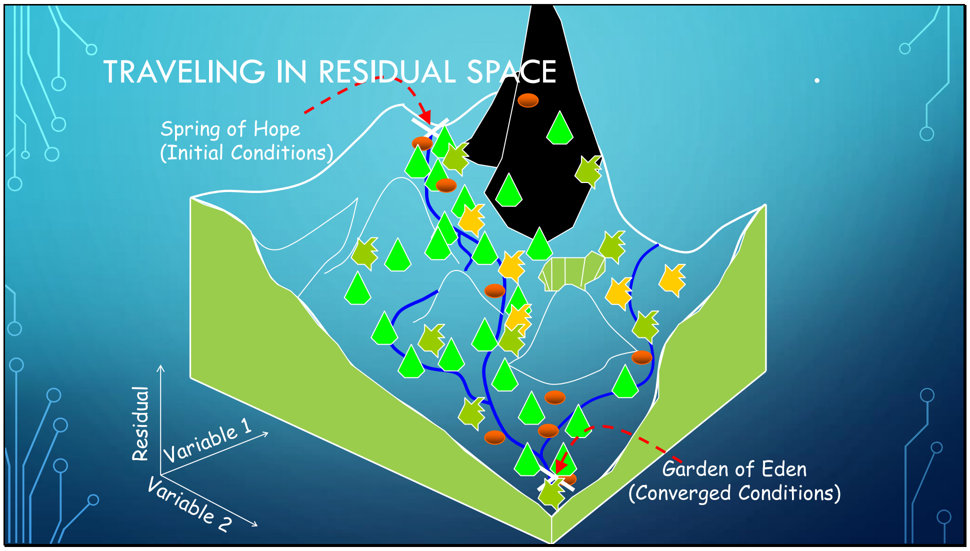

TRAVELING IN RESIDUAL SPACE

Creating a solution to the governing equations as analogous to getting water from a spring in the mountains to a pool in the a valley below. The water's position at the begging is like our initial conditions (out initial guess for the solution) and the position at the pool is our converged condition (where all the equations are satisfied). High in the mountains, our residual (error) is high. At the pool our residual is zero.

The first thing to note is that there are many possible ways for the water to get from the spring to the pool. It can flow in a river or be carried in a helicopter. These represent alternate solution paths. There are also many possible springs that can reach the pool. These represent alternate initial conditions.

Also note that all we care about is getting to the pool. The trip through the forest is not the important thing. If we could carry the water in a helicopter from the spring to the pool, that is fine. The problem is, we have to know where it is.

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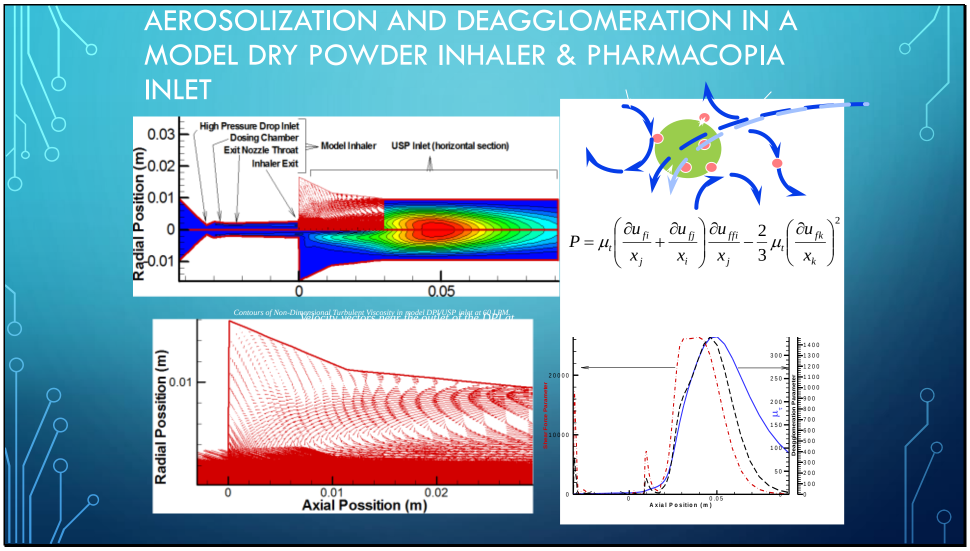


AEROSOLIZATION AND DEAGGLOMERATION IN A MODEL DRY POWDER INHALER & PHARMACOPIA INLET

$$P = \mu_t \left(\frac{\partial u_{fi}}{x_j} + \frac{\partial u_{fj}}{x_i} \right) \frac{\partial u_{ffi}}{x_j} - \frac{2}{3} \mu_t \left(\frac{\partial u_{fk}}{x_k} \right)^2$$

Contours of Non-Dimensional Turbulent Viscosity in model DPI/USP inlet at 60 LPM.

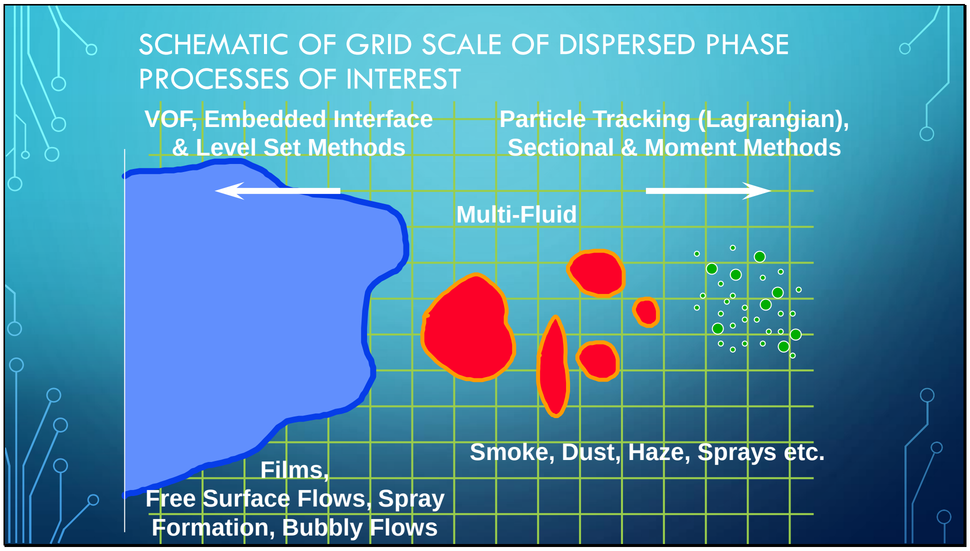
Velocity vectors near the outlet of the DPI at

A coupled 2-D / Axisymmetric / 3-D flow and moment model incorporating the effects of nucleation, condensation, coagulation, diffusion, inertial impaction and thermophoresis has been developed. Computations have been presented with and RNS / aerosol model in general non-orthogonal coordinates for a variety of flows. The method has been shown to provide meaningful data on the complex behavior of aerosols under these flow conditions.

A sample calculation of NASA's Variable Diameter Inlet geometry was used to demonstrate the capabilities of the flow module. In this complex, unsteady, turbulent geometry, the RNS methodology is found to accurately compute separation regions, normal and oblique shocks for internal \ external flow regions. The capabilities of the aerosol transport module have been demonstrated in a 3-D 180° turnaround duct. Complex flow-aerosol interactions are detailed. An analysis of gas to particle conversion in an incompressible to supersonic converging diverging nozzle demonstrates the detailed particle dynamics that can be modeled using this method. Preliminary results indicate the importance of multidimensionality in determining aerosol behavior in such geometries. Discrepancies between average or integrated values of aerosol properties in 2-D calculations can be as much as 10% as compared to 1-D calculations. Initial results indicate that the effects of aerosol dynamics on flow conditions are small for the relatively low conversion rates investigated. Validation of these results is ongoing. Analysis aerosol behavior shows the importance of correctly modeling all aspects of gas to particle conversion. For instance, it is shown that neglecting the nucleation process, even when seed particles are present, can result is large under-prediction of resultant aerosol volume concentrations and erroneous size distributions.   A detailed analysis of aerosol effects on the flow is ongoing.

It has been demonstrated that the present moment model is effective and efficient in solving for the complex behavior of polydisperse aerosols in general flow applications. Many important aerosol properties, such as size distributions, number and volume concentrations and depositional properties, can be calculated directly without having to sum up results for monodisperse aerosols over the entire particle spectrum. Research is presently underway to perform coupled flow and aerosol simulations under turbulent conditions in nozzles, plumes and inlets.

Modelling



SCHEMATIC OF GRID SCALE OF DISPERSED PHASE PROCESSES OF INTEREST

VOF, Embedded Interface & Level Set Methods

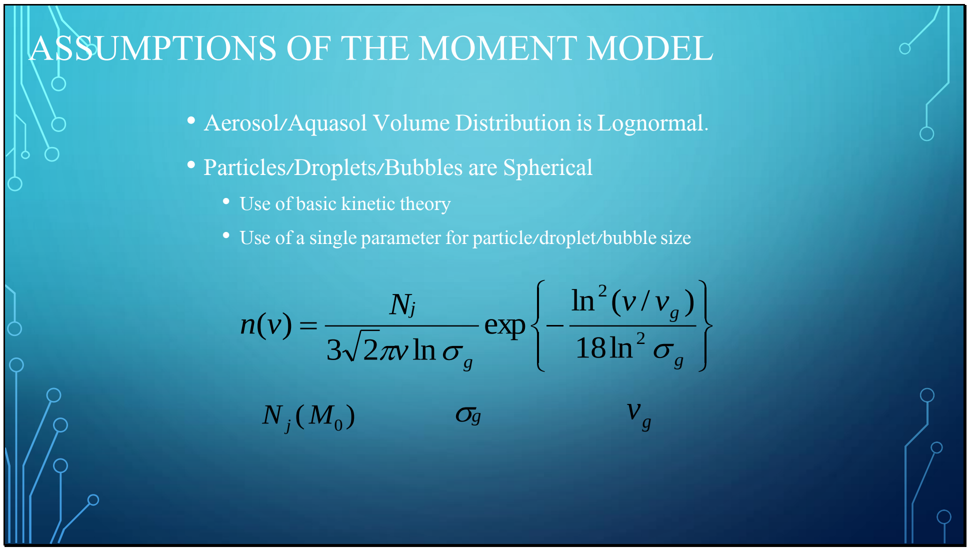
Particle Tracking (Lagrangian), Sectional & Moment Methods

Multi-Fluid

Smoke, Dust, Haze, Sprays etc.

Films,
Free Surface Flows, Spray Formation, Bubbly Flows

Dynamic mechanisms such as coagulation, nucleation and condensation can become important in many instances. These mechanisms help define the chemical composition of the aerosols as well as effecting aerosol transport, polydispersisity effects and gas phase species concentration. A schematic of aerosol dynamic mechanisms is shown here. The process can begin either in the gas phase, through seed particles, or through generation via chemical reactions. Gas phase species can also nucleate to form aerosols. These aerosols can then grow through condensation of gas phase species on existing particles or trough coagulation of existing particles.



ASSUMPTIONS OF THE MOMENT MODEL

- Aerosol/Aquasol Volume Distribution is Lognormal.
- Particles/Droplets/Bubbles are Spherical
  - Use of basic kinetic theory
  - Use of a single parameter for particle/droplet/bubble size

$$n(v) = \frac{N_j}{3\sqrt{2}\pi v \ln \sigma_g} \exp\left\{ -\frac{\ln^2(v/v_g)}{18\ln^2 \sigma_g} \right\}$$

$N_j(M_0)$ σ_g v_g

Several simplifying assumptions were made to make the model more manageable without losing a great deal of generality.

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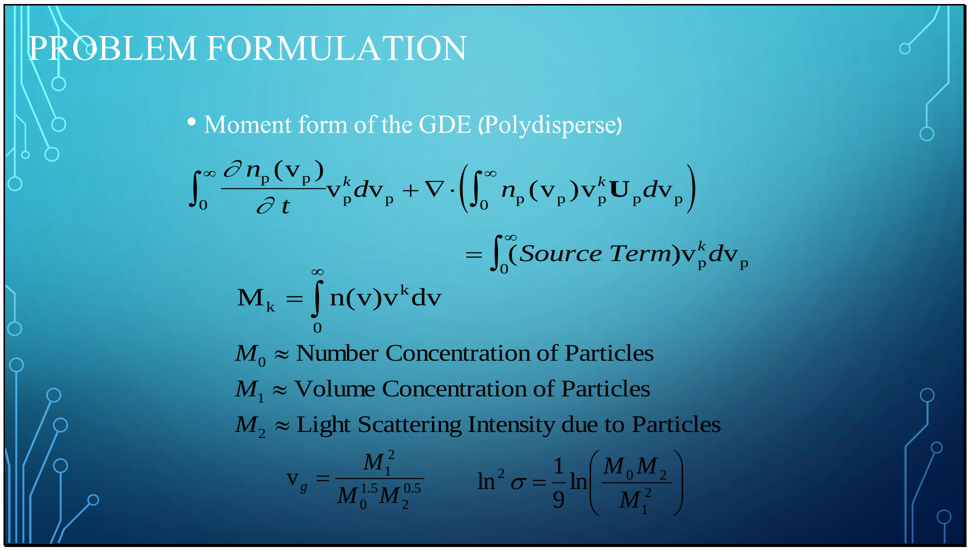

PROBLEM FORMULATION

- Moment form of the GDE (Polydisperse)

$$\int_0^\infty \frac{\partial n_\mathrm{p}(\mathrm{v}_\mathrm{p})}{\partial t}\mathrm{v}_\mathrm{p}^k d\mathrm{v}_\mathrm{p} + \nabla\cdot\left(\int_0^\infty n_\mathrm{p}(\mathrm{v}_\mathrm{p})\mathrm{v}_\mathrm{p}^k \mathbf{U}_\mathrm{p} d\mathrm{v}_\mathrm{p}\right)$$

$$= \int_0^\infty (Source\ Term)\mathrm{v}_\mathrm{p}^k d\mathrm{v}_\mathrm{p}$$

$$\mathrm{M_k} = \int_0^\infty \mathrm{n(v)v^k dv}$$

$M_0 \approx$ Number Concentration of Particles

$M_1 \approx$ Volume Concentration of Particles

$M_2 \approx$ Light Scattering Intensity due to Particles

$$\mathrm{v}_g = \frac{M_1^2}{M_0^{1.5} M_2^{0.5}} \qquad \ln^2\sigma = \frac{1}{9}\ln\left(\frac{M_0 M_2}{M_1^2}\right)$$

k*/=number of molecules in a critical cluster
ns = number of molecules in cluster at saturation

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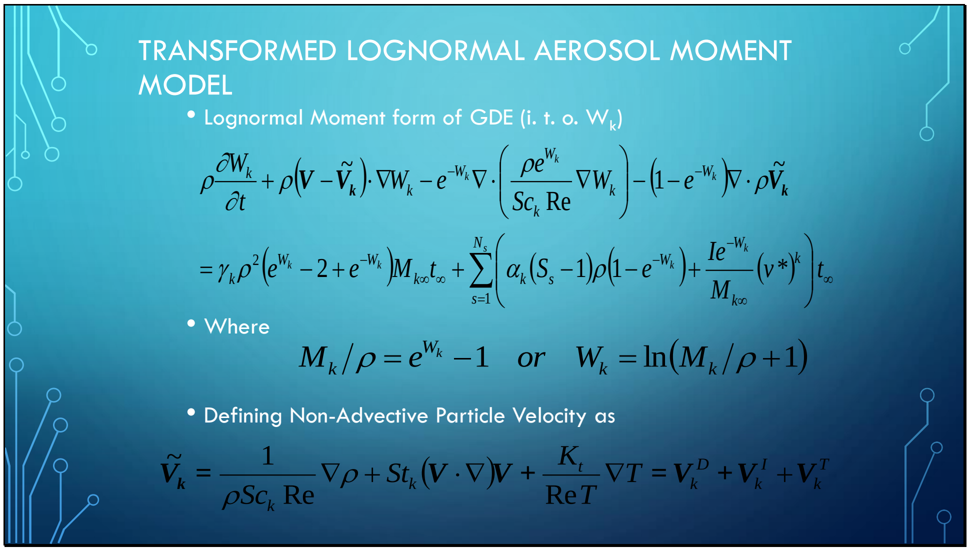

TRANSFORMED LOGNORMAL AEROSOL MOMENT MODEL

- Lognormal Moment form of GDE (i. t. o. W_k)

$$\rho\frac{\partial W_k}{\partial t}+\rho\left(\mathbf{V}-\tilde{\mathbf{V}}_{\boldsymbol{k}}\right)\cdot\nabla W_k-e^{-W_k}\nabla\cdot\left(\frac{\rho e^{W_k}}{Sc_k\,\mathrm{Re}}\nabla W_k\right)-\left(1-e^{-W_k}\right)\nabla\cdot\rho\tilde{\mathbf{V}}_{\boldsymbol{k}}$$

$$=\gamma_k\rho^2\left(e^{W_k}-2+e^{-W_k}\right)M_{k\infty}t_\infty+\sum_{s=1}^{N_s}\left(\alpha_k\left(S_s-1\right)\rho\left(1-e^{-W_k}\right)+\frac{Ie^{-W_k}}{M_{k\infty}}\left(v^*\right)^k\right)t_\infty$$

- Where

$$M_k/\rho=e^{W_k}-1\quad or\quad W_k=\ln\left(M_k/\rho+1\right)$$

- Defining Non-Advective Particle Velocity as

$$\tilde{\mathbf{V}}_{\boldsymbol{k}}=\frac{1}{\rho Sc_k\,\mathrm{Re}}\nabla\rho+St_k\left(\mathbf{V}\cdot\nabla\right)\mathbf{V}+\frac{K_t}{\mathrm{Re}\,T}\nabla T=\mathbf{V}_k^D+\mathbf{V}_k^I+\mathbf{V}_k^T$$

In several of the cases gradients in Mk were very large. These gradients sometimes caused difficulties in obtaining the the numerical solution of the governing equations in terms of the moments Mk due to, essentially, shocks or discontinuities.
To alleviate this problem the aerosol governing equations were recast in terms of the a transformed variable Wk which is related to the original variable Mk through the mapping Mk/r-exp(Wk)-1. This transformed formulation has several advantages over the original formulation namely, the range of Wk is smaller (typically ranging from 0 to 50 as opposed to 0 to 1x10 ??) reducing the magnitude of gradients. As well, Wk is a conserved variable. Thus, if there are no particle dynamics or transport (other than convection) present, Wk is constant, even in a compressible flow. The main disadvantage is the the increased complexity (and non-linearity) or the RHS source terms.